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NEWS	1			Web Page for STN Seminar Schedule - N. America
NEWS		DEC	01	
NEWS	3	APR	03	CAS coverage of exemplified prophetic substances enhanced
NEWS	Α	ADD	0.7	STN is raising the limits on saved answers
NEWS			24	
MEMO	J	MER	24	information
NEWS	6	APR	26	USPATFULL and USPAT2 enhanced with patent assignment/reassignment information
NEWS	7	APR	28	
NEWS				
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				REGISTRY
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NEWS				
NEWS	12	MAY	11	BEILSTEIN substance information now available on STN Easy
NEWS	13	MAY	14	DGENE, PCTGEN and USGENE enhanced with increased
NEWS	1.4	143.14	16	limits for exact sequence match searches and introduction of free HIT display format INPADOCDB and INPAFAMDB enhanced with Chinese legal
MEMP	14	PIAI	10	status data
NEWS	15	MAV	28	
HEND	10		20	records back to 1992
NEWS	16	JUN	01	CAS REGISTRY Source of Registration (SR) searching
		0 011	0.2	enhanced on STN
NEWS	17	JUN	26	
NEWS			29	
NEWS			29	EPFULL adds Simultaneous Left and Right Truncation
				(SLART) to AB, MCLM, and TI fields
NEWS	20	JUI.	0.9	
				Truncation (SLART) to AB, CLM, MCLM, and TI fields
NEWS	21	JUL	14	USGENE enhances coverage of patent sequence location
NEWS	22	TITY	14	(PSL) data CA/CAplus to be enhanced with new citing references
				features
NEWS	23			GBFULL adds patent backfile data to 1855
NEWS	24	JUL	21	USGENE adds bibliographic and sequence information
NEWS	EXPI	RESS		26 09 CURRENT WINDOWS VERSION IS V8.4, CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.

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FILE 'HOME' ENTERED AT 12:22:34 ON 21 JUL 2009

Uploading

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=> FILE REGISTRY

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FULL ESTIMATED COST

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http://www.cas.org/support/stngen/stndoc/properties.html

Uploading C:\Program Files\Stnexp\Queries\10591774.str

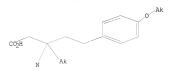
chain nodes : 7 8 9 10 11 12 13 14 16 ring nodes : 1 2 3 4 5 6 chain bonds : 2-7 5-14 7-8 8-9 9-10 9-12 9-13 10-11 14-16 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 exact/norm bonds : 5-14 9-12 9-13 14-16 exact bonds : 2-7 7-8 8-9 9-10 10-11 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 isolated ring systems : containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 16:CLASS

L1 STRUCTURE UPLOADED

=> D L1 L1 HAS NO ANSWERS L1 STR



Structure attributes must be viewed using STN Express query preparation.

10591774.trn 07/21/2009 Page 3

=> S L1

SAMPLE SEARCH INITIATED 12:23:11 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 119 TO ITERATE

100.0% PROCESSED 119 ITERATIONS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

0 ANSWERS

BATCH **COMPLETE** PROJECTED ITERATIONS: 1726 TO 3034 0 TO

PROJECTED ANSWERS:

0 SEA SSS SAM L1

=> S L1 SSS FULL

FULL SEARCH INITIATED 12:23:19 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 2403 TO ITERATE

100.0% PROCESSED 2403 ITERATIONS 1 ANSWERS

SEARCH TIME: 00.00.01

1 SEA SSS FUL L1

=> FIL HCAPLUS

SINCE FILE TOTAL ENTRY SESSION COST IN U.S. DOLLARS FULL ESTIMATED COST 185.88 186.10

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FILE COVERS 1907 - 21 Jul 2009 VOL 151 ISS 4 FILE LAST UPDATED: 20 Jul 2009 (20090720/ED) REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2009 USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2009

HCAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2009.

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10591774.trn 07/21/2009 Page 4

This file contains CAS Registry Numbers for easy and accurate substance identification.

The ALL, BIB, MAX, and STD display formats in the CA/CAplus family of databases will soon be updated to include new citing references information. This enhancement may impact record import into database management software. For additional information, refer to NEWS 25.

=> S L3 L4 1 L3

=> d l4 ibib abs hitstr tot

L4 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:1004693 HCAPLUS DOCUMENT NUMBER: 143:267240

DOCUMENT NUMBER: 143:26724 TITLE: Preparati

TITLE: Preparation of amino acid derivatives and pharmaceutical compositions containing them

INVENTOR(S): Hinterding, Klaus; Hoegenauer, Klemens
PATENT ASSIGNEE(S): Novartis A.-G., Switz.; Novartis Pharma G.m.b.H.

SOURCE: PCT Int. Appl., 24 pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PA: | TENT | NO. | | | KIN | KIND DATE | | APPLICATION NO. | | | | | DATE | | | | | |
|-----|---------------|------|-----|-----|-----|------------|------|-----------------|-----------------|---------------------------------------|----------------|-------|------|-----|----------|------|------|----|
| WO | WO 2005085179 | | | | A1 | - | 2005 | 0915 | | | | | | | 2 | 0050 | 308 | |
| | W: | ΑE, | AG, | AL, | AM, | AT, | AU, | AZ, | BA, | BB, | BG, | BR, | BW, | BY, | BZ, | CA, | CH, | |
| | | CN, | CO, | CR, | CU, | CZ, | DE, | DK, | DM, | DZ, | EC, | EE, | EG, | ES, | FI, | GB, | GD, | |
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| AU | U 2005219562 | | | | A1 | . 20050915 | | | AU 2005-219562 | | | | | | 2 | 0050 | 308 | |
| AU | 2005219562 | | | | B2 | | 2008 | 1016 | | | | | | | | | | |
| CA | 2558 | 167 | | | A1 | . 20050915 | | | CA 2005-2558167 | | | | | | 20050308 | | | |
| EP | | | | | | | | | | EP 2005-715843
DK, EE, ES, FI, FR, | | | | | | | | |
| | R: | | | | | | | | | | | | | | | | IE, | |
| 011 | 1001 | | | | | | | | | | RO, | | | | | | 200 | |
| CIN | 1934 | 069 | | | A | | 2007 | 0321 | | UN Z | 2005- | 8000 | 95/5 | | 2 | 0050 | 308 | |
| BR | 2005 | 0086 | 10 | | A | | 2007 | 1000 | | BR 2 | 2005-
2007- | 8610 | 20 | | 2 | 0050 | 308 | |
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| 05 | 2007 | 0133 | 201 | | AI | | 2007 | 0014 | | 05 2 | -000- | JJ1 / | / 11 | | 2 | 0001 | 0.10 | |

PRIORITY APPLN. INFO.:

GB 2004-5289 A 20040309 WO 2005-EP2447 W 20050308

OTHER SOURCE(S): CASREACT 143:267240: MARPAT 143:267240

AB The invention relates to new amino acid derivs. R4RSNCRIR3CH2CH2R2 [R1 is alkyl optionally substituted by OH, alkoxy or F, alkenyl, alkynyl, R2 is R6X-substituted Ph (may be further substituted) or 2-naphthyl.
2-R6X-substituted benzoxazol-5-yl or benzodioxol-5-yl, where X is O, CO, S or a bond and R6 is optionally substituted alkyl or oxa- or oxoalkyl; R3 is -A-B-CO2H, where A and B are independently a bond, CO or CDE (D and E are independently H, halo or alkyl); R4, R5 are independently H, haloalkyl or acyl (with provisos)], including their production and use, particularly in transplantation. Thus,

(R)-3-amino-5-[4-(heptyloxy)phenyl]-3-methylpentanoic acid, prepared by a multistep sequence starting from N-Boc-protected

(R)-2-amino-4-(4-hydroxyphenyl)-2-methyl-1-butanol, showed binding affinity to individual human sphingosine 1 phosphate (S1P) receptors (EC50 for binding to S1P1 is 11 nM).

863991-32-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of amino acid derivs. and pharmaceutical compns. containing them)

RN 863991-32-6 HCAPLUS

CN Benzenepentanoic acid, β-amino-4-(heptyloxy)-β-methyl-, (βR)- (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> FIL REGISTRY COST IN U.S. DOLLARS FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 17.04 203.14

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL ENTRY SESSION -0.82 -0.82

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chain nodes : 7 8 9 10 11 12 13 ring nodes : 1 2 3 4 5 6 chain bonds : 2-7 7-8 8-9 9-10 9-12 9-13 10-11 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 exact/norm bonds : 9-12 9-13 exact bonds : 2-7 7-8 8-9 9-10 10-11 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 isolated ring systems : containing 1:

Match level: 1:Atom 2:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS

L5 STRUCTURE UPLOADED

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10591774.trn 07/21/2009



Structure attributes must be viewed using STN Express query preparation.

=> s 15

SAMPLE SEARCH INITIATED 12:26:13 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED -302 TO ITERATE

302 ITERATIONS 6 ANSWERS 100.0% PROCESSED SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE** **COMPLETE** BATCH PROJECTED ITERATIONS: 4998 TO 7082 PROJECTED ANSWERS: 6 TO 266

6 SEA SSS SAM L5 1.6

=> s 15 sss full

FULL SEARCH INITIATED 12:26:21 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED -6074 TO ITERATE

100.0% PROCESSED 6074 ITERATIONS 68 ANSWERS SEARCH TIME: 00.00.01

68 SEA SSS FUL L5

=> FIL HCAPLUS

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION 186.36 FULL ESTIMATED COST 389.50 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL. SESSION ENTRY

CA SUBSCRIBER PRICE 0.00 -0.82

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FILE COVERS 1907 - 21 Jul 2009 VOL 151 ISS 4 FILE LAST UPDATED: 20 Jul 2009 (20090720/ED) REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2009 USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2009

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=> d his

(FILE 'HOME' ENTERED AT 12:22:34 ON 21 JUL 2009)

FILE 'REGISTRY' ENTERED AT 12:22:56 ON 21 JUL 2009 STRUCTURE UPLOADED

L2 0 S L1

L3 1 S L1 SSS FULL

FILE 'HCAPLUS' ENTERED AT 12:23:25 ON 21 JUL 2009 T. 4 1 5 1.3

FILE 'REGISTRY' ENTERED AT 12:25:32 ON 21 JUL 2009 STRUCTURE UPLOADED

FILE 'HCAPLUS' ENTERED AT 12:26:49 ON 21 JUL 2009

L5 1.6 6 S L5 68 S L5 SSS FULL

=> s 176 L7

L8

=> d 18 ibib abs hitstr tot

L8 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 2008:525259 HCAPLUS

DOCUMENT NUMBER: 148:585420

TITLE: A New Silicon Lewis Acid for Highly Enantioselective Mannich Reactions of Aliphatic Ketone-Derived

Hydrazones

AUTHOR(S): Notte, Gregory T.; Leighton, James L.

CORPORATE SOURCE: Department of Chemistry, Columbia University, New York, NY, 10027, USA

Journal of the American Chemical Society (2008), SOURCE:

130(21), 6676-6677

CODEN: JACSAT: ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 148:585420

The first general method for the highly enantioselective Mannich reaction AB of aliphatic ketimines is reported. A new, second generation chiral silane Lewis acid has been developed that promotes the reaction between ketone-derived hydrazones and silyl ketene acetals, providing the β , β -disubstituted β -amino esters, e.g., I, with good enantioselectivity even for the hydrazone derived from 2-butanone (Me vs Et, 91% ee). Several examples are provided, including a reaction with a substituted (propanoate-derived) silyl ketene acetal.

1028492-27-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (crystal structure; stereoselective preparation of (tetrahydroquinolinyl)acetate derivative via chiral silane-catalyzed enantioselective Mannich reaction, reduction, and heterocyclization of (bromophenyl)butanone-derived hydrazone)

RN 1028492-27-4 HCAPLUS

Benzenepentanoic acid, 2-bromo-β-methyl-β-[(4-CN nitrobenzovl)aminol-, (BS)- (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2007:1201261 HCAPLUS DOCUMENT NUMBER: 148:54432

TITLE: Asymmetric formation of allylic amines with

N-substituted quaternary stereocenters by PdII-catalyzed aza-Claisen rearrangements AUTHOR(S): Fischer, Daniel F.; Xin, Zhuo-qun; Peters, Rene

CORPORATE SOURCE: Laboratory of Organic Chemistry, ETH Zuerich, Zurich, 8093, Switz.

SOURCE: Angewandte Chemie, International Edition (2007),

46(40), 7704-7707

CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

PUBLISHER: Wiley-VCH Verlag GmbH & Co

LANGUAGE: English

OTHER SOURCE(S): CASREACT 148:54432

AB With (u-Cl)2[Pd(2-((4R,SR)-4,5-di-tert-butyl-4,5-dihydro-1-tosyl-lHimidazol-2-yl-1-1;2,'3,'4,'5-pentaphenylferrocenyl)]2 (containing 1 diastereomer of the ligand) as precatalyst, quaternary N-substituted stereocenters can be generated in an asym. aza-Claisen rearrangement. Excellent enantioselectivities were obtained even if R and R' have a similar or identical size (e.g. 96% ee for CH3/CD3, i.e. conversion of (E)-MeC(CD3):CHCH2CC(CF3):NPMP to (R)-CF3C(O) N(PMP)CME (CD3):CH3(CB).

IT 960060-26-8P, (R)-3-[[[(9H-Fluoren-9-y1)methoxy]carbonyl]amino]-3methyl-5-phenylpentanoic acid

RL: SPN (Synthetic preparation); PREP (Preparation) (asym. formation of allylic amines with N-substituted quaternary stereocenters by PdII-catalyzed aza-Claisen rearrangements)

RN 960060-26-8 HCAPLUS

CN Benzenepentanoic acid, β-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]β-methyl-, (βR)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 2005:1004693 HCAPLUS DOCUMENT NUMBER: 143:267240

INVENTOR(S):

LANGUAGE:

TITLE:

Preparation of amino acid derivatives and pharmaceutical compositions containing them Hinterding, Klaus; Hoegenauer, Klemens

ADDITORTION NO

DATE

PATENT ASSIGNEE(S): Novartis A.-G., Switz.; Novartis Pharma G.m.b.H. SOURCE: PCT Int. Appl., 24 pp.

English

KIND DATE

CODEN: PIXXD2 DOCUMENT TYPE: Patent

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION: DATENT NO

| PA | TENT | NO. | | | KIN | D | DATE | | | APPL | ICAT | ION | NO. | | D. | ATE | | |
|---------|------------|--------|------|-----|-----|---|------|------|-----|-------|------|-------|-----|-----|------|-------|-----|----|
| WC | 2005 | 0851 | 79 | | A1 | _ | 2005 | 0915 | | WO 2 | 005- | EP24 | 47 | | 2 | 0050 | 308 | |
| | W: | ΑE, | AG, | AL, | AM, | AT, | AU, | AZ, | BA, | BB, | BG, | BR, | BW, | BY, | BZ, | CA, | CH, | |
| | | CN, | co, | CR, | CU, | CZ, | DE, | DK, | DM, | DZ, | EC, | EE, | EG, | ES, | FI, | GB, | GD, | |
| | | GE, | GH, | GM, | HR, | HU, | ID, | IL, | IN, | IS, | JP, | KE, | KG, | KP, | KR, | KZ, | LC, | |
| | | LK, | LR, | LS, | LT, | LU, | LV, | MA, | MD, | MG, | MK, | MN, | MW, | MX, | MZ, | NA, | NI, | |
| | | NO, | NZ, | OM, | PG, | PH, | PL, | PT, | RO, | RU, | SC, | SD, | SE, | SG, | SK, | SL, | SM, | |
| | | SY, | TJ, | TM, | TN, | TR, | TT, | TZ, | UA, | UG, | US, | UZ, | VC, | VN, | YU, | ZA, | ZM, | ZW |
| | RW: | BW, | GH, | GM, | KE, | LS, | MW, | MZ, | NA, | SD, | SL, | SZ, | TZ, | UG, | ZM, | ZW, | AM, | |
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| | | | | | TD, | | | | | | | | | | | | | |
| AU | 2005 | 2195 | 62 | | A1 | | 2005 | 0915 | | AU 2 | 005- | 2195 | 62 | | 2 | 0050 | 308 | |
| AU | 2005 | 2195 | 62 | | B2 | | 2008 | 1016 | | | | | | | | | | |
| CA | 2558 | 167 | | | A1 | | 2005 | 0915 | | CA 2 | 005- | 2558 | 167 | | 2 | 0050 | 308 | |
| EP | EP 1725519 | | | | | 20061129 EP 2005-715843 200
Y, CZ, DE, DK, EE, ES, FI, FR, GB, GR, H | | | | | | | | | | | | |
| | R: | | | | | | | | | | | | | | | | IE, | |
| | | | | | | | MC, | | | | | | | | | | | |
| | 1934 | | | | | | 2007 | | | | | | | | | | | |
| BH | 2005 | 0086 | 10 | | A | | 2007 | 0/31 | | BR Z | 005- | 8610 | 20 | | 2 | 0050 | 308 | |
| JE | 2007 | 5354 | 99 | | 1 | | 2007 | 1206 | | JP Z | 007- | 5022 | 19 | | 2 | 0050 | 308 | |
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| | 2006 | | | | | | | | | | | | | | | | | |
| | 2007 | | | | | | | | | KK Z | 006- | /183 | 44 | | 2 | 0060 | 908 | |
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| | | | | | | | | | | WU Z | 000- | DF 24 | 4 / | | ve Z | 0030. | 200 | |

OTHER SOURCE(S): CASREACT 143:267240: MARPAT 143:267240

The invention relates to new amino acid derivs. R4R5NCR1R3CH2CH2R2 [R1 is alkyl optionally substituted by OH, alkoxy or F, alkenyl, alkynyl; R2 is R6X-substituted Ph (may be further substituted) or 2-naphthyl, 2-R6X-substituted benzoxazol-5-yl or benzodioxol-5-yl, where X is O, CO, S or a bond and R6 is optionally substituted alkyl or oxa- or oxoalkyl; R3 is -A-B-CO2H, where A and B are independently a bond, CO or CDE (D and E are independently H, halo or alkyl); R4, R5 are independently H, alkyl, haloalkyl or acyl (with provisos)], including their production and use, particularly in transplantation. Thus,
(R)-3-amino-5-[4-(heptyloxy)phenyl]-3-methylpentanoic acid, prepared by a

- multistep sequence starting from N-Boc-protected
- (R)-2-amino-4-(4-hydroxyphenyl)-2-methyl-1-butanol, showed binding affinity to individual human sphingosine 1 phosphate (S1P) receptors (EC50 for binding to SIP1 is 11 nM).
- 863991-32-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of amino acid derivs. and pharmaceutical compns. containing

them) RN 863991-32-6 HCAPLUS

REFERENCE COUNT:

Benzenepentanoic acid, β-amino-4-(heptvloxv)-β-methvl-, CN (BR) - (CA INDEX NAME)

Absolute stereochemistry.

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 2005:426562 HCAPLUS

DOCUMENT NUMBER: 142:481829

TITLE: Preparation of amino(phenyl)alkanoic acid derivatives, addition salts thereof, and sphingosine-1-phosphate

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS

(S1P) receptor modulators

INVENTOR(S): Kohno, Yasushi; Tanioka, Sayoko; Kikuchi, Yoshiaki; Kinoshita, Miki; Iwanami, Satoru

PATENT ASSIGNEE(S): Kyorin Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 221 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent. LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT NO. | KIND DATE | APPLICATION NO. | DATE | | | | | | | |
|------------------------|-------------------|---------------------|-----------------|--|--|--|--|--|--|--|
| WO 2005044780 | 31 20050510 | WO 2004-JP16517 | 20041100 | | | | | | | |
| | | | | | | | | | | |
| W: AE, AG, AL, | AM, AT, AU, AZ, | BA, BB, BG, BR, BW, | BY, BZ, CA, CH, | | | | | | | |
| | | DM, DZ, EC, EE, EG, | | | | | | | | |
| GE, GH, GM, | HR, HU, ID, IL, | IN, IS, JP, KE, KG, | KP, KR, KZ, LC, | | | | | | | |
| LK, LR, LS, | LT, LU, LV, MA, | MD, MG, MK, MN, MW, | MX, MZ, NA, NI, | | | | | | | |
| NO, NZ, OM, | PG, PH, PL, PT, | RO, RU, SC, SD, SE, | SG, SK, SL, SY, | | | | | | | |
| TJ, TM, TN, | TR, TT, TZ, UA, | UG, US, UZ, VC, VN, | YU, ZA, ZM, ZW | | | | | | | |
| RW: BW, GH, GM, | KE, LS, MW, MZ, | NA, SD, SL, SZ, TZ, | UG, ZM, ZW, AM, | | | | | | | |
| AZ, BY, KG, | KZ, MD, RU, TJ, | TM, AT, BE, BG, CH, | CY, CZ, DE, DK, | | | | | | | |
| EE, ES, FI, | FR, GB, GR, HU, | IE, IS, IT, LU, MC, | NL, PL, PT, RO, | | | | | | | |
| SE, SI, SK, | TR, BF, BJ, CF, | CG, CI, CM, GA, GN, | GQ, GW, ML, MR, | | | | | | | |
| NE, SN, TD, | TG | | A 20031110 | | | | | | | |
| PRIORITY APPLN. INFO.: | | JP 2003-380383 | | | | | | | | |
| OTHER SOURCE(S): | MARPAT 142:481829 | | | | | | | | | |

10591774.trn 07/21/2009

AB

[wherein R1 = each (un) substituted Ph or C1-10 alkyl; R2 = H, halo, trihalomethyl, C1-4 alkyl, C1-4 alkoxy; R3 = H, C1-4 alkyl, Ph; R4 = H, (un) substituted C1-4 alkyl, C2-4 alkenyl, C2-4 alkynyl, CO2H, C1-4 alkoxycarbonyl, benzyloxycarbonyl, CH2OCH2CO2H, CH2OCH2CO2R6 (wherein R6 = C1-4 alkyl, benzyl); X = 0, S, SO, SO2; m = 2-4; Y = CH:CH, CH2OCH2, (CH2) n (wherein n = an integer of 0-2), CH2OCHCO2R5 (R5 = same as above)], optical isomers, pharmacol. acceptable salts, or hydrates thereof are prepared These compds. are highly effective in controlling a sphingosine-1-phosphoric acid (S1P) receptor. For example, 3-amino-6-(4-(3-benzyloxyphenylsulfanyl)-2-chlorophenyl]-3hydroxymethylhexanoic acid induced the cellular calcium uptake in CHO cells expressing human S1P1 receptor and those expressing human S1P3 receptor with ED50 of <1 µmol and ≥10 µM, resp. The compds. I in vitro induced the activation of extracellular regulatory kinase in CHO cells expressing human S1P receptor and in vivo inhibited the host-vs.-graft rejection in transplant of lymph node in mice. 852053-21-5P 852055-44-8P, ΙT 3-Amino-5-[4-[(4-benzyloxyphenyl)thio]-2-chlorophenyl]-3hydroxymethylpentanoic acid 852055-46-0P, 3-Amino-5-[4-[(4-benzyloxyphenyl)thio]-2-chlorophenyl]-3-(3hydroxypropyl)pentanoic acid 852055-48-2P, 3-Amino-5-[4-[(4-benzyloxyphenyl)thio]-2-chlorophenyl]-3-propylpentanoic

Aminocarboxylic acid derivs, represented by the general formula (I)

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (extracellular-regulatory kinase activation inducers; preparation of amino(phenyl)alkanoic acid derivs. as sphingosine-1-phosphate (S1P) receptor modulators)

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

- RN 852053-21-5 HCAPLUS
- CN Benzenepentanoic acid, β-amino-2-chloro-β-(hydroxymethyl)-4-[[3-(phenylmethoxy)phenyl]thio]- (CA INDEX NAME)

acid 852055-50-6P, 3-Allyl-3-amino-5-[4-[(4-benzyloxyphenyl)thio]-2-chlorophenyl]pentanoic acid

- RN 852055-44-8 HCAPLUS
- CN Benzenepentanoic acid, β-amino-2-chloro-β-(hydroxymethyl)-4-[[4-

10591774.trn 07/21/2009 Page 14

(phenylmethoxy)phenyl]thio]- (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \text{NH}_2 \\ \text{HO}_2\text{C-}\text{CH}_2\text{-}\text{C-}\text{CH}_2\text{-}\text{CH}_2 \\ \text{HO-}\text{CH}_2 \end{array} \\ \begin{array}{c} \text{C1} \\ \text{S-}\text{CH}_2\text{-}\text{Ph} \\ \text{CH}_2\text{-}\text{Ph} \end{array}$$

- RN 852055-46-0 HCAPLUS
- CN Benzenepentanoic acid, β-amino-2-chloro-β-(3-hydroxypropyl)-4-[[4-(phenylmethoxy)phenyl]thio]- (CA INDEX NAME)

- RN 852055-48-2 HCAPLUS
- CN Benzenepentanoic acid, β-amino-2-chloro-4-[[4-(phenylmethoxy)phenyl]thio]-β-propyl- (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \text{HO}_2\text{C}-\text{CH}_2 \\ \text{n-Pr}-\text{C-CH}_2-\text{CH}_2 \\ \text{NH}_2 \end{array}$$

- RN 852055-50-6 HCAPLUS
- CN Benzenepentanoic acid, β-amino-2-chloro-4-[[4-(phenylmethoxy)phenyl]thio]-β-2-propen-1-yl- (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \text{NH}_2 \\ \text{H}_2\text{C} = \text{CH} - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\ \text{HO}_2\text{C} - \text{CH}_2 - \text{CH}_2 \end{array}$$

IT 852053-22-6P 852053-25-9P 852053-28-2P 852053-35-1P 852053-39-5P 852053-40-8P 852053-41-9P 852053-68-0P 852053-69-1P

852053-89-5P 852053-90-8P 852053-91-9P 852054-08-1P 852054-10-5P 852054-12-7P 852054-14-9P 852054-43-4P 852054-45-6P 852054-46-7P 852054-48-9P 852054-50-3P 852054-52-5P 852054-84-3P 852054-86-5P 852054-88-7P 852054-91-2P 852054-93-4P 852054-95-6P 852054-97-8P 852054-99-0P 852055-01-7P 852055-03-9P 852055-05-1P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of amino(phenyl)alkanoic acid derivs. as sphingosine-1-phosphate (S1P) receptor modulators) 852053-22-6 HCAPLUS

RN

CM Benzenepentanoic acid, β-amino-2-chloro-β-(hydroxymethyl)-4-[[3-(phenylmethoxy)phenyl]thio]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} & \text{C} \\ \text{NH}_2 & \text{C} \\ \text{HO}_2 \text{C} - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\ \text{HO} - \text{CH}_2 & \text{CH}_2 \end{array}$$

HC1

852053-25-9 HCAPLUS RN

CN Benzenepentanoic acid, β-amino-2-chloro-β-(hydroxymethyl)-4-[3-(trifluoromethyl)phenoxy] - (CA INDEX NAME)

RN 852053-28-2 HCAPLUS

CN Benzenepentanoic acid, β-amino-2-chloro-β-(hydroxymethyl)-4-[[4-(phenylmethoxy)phenyl]thio]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \text{NH}_2 \\ \text{HO}_2\text{C}-\text{CH}_2-\text{C}-\text{CH}_2-\text{CH}_2 \\ \text{HO}-\text{CH}_2 \end{array}$$

- RN 852053-35-1 HCAPLUS
- CN Benzenepentanoic acid, β-amino-β-(hydroxymethyl)-4-octyl-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} & \text{NH}_2 \\ & \text{HO}_2\text{C-CH}_2\text{-C-CH}_2\text{-CH}_2 \\ & \text{HO-CH}_2 \end{array}$$

● HCl

- RN 852053-39-5 HCAPLUS
- CN Benzenepentanoic acid, β-amino-2-chloro-4-[[3-(phenylmethoxy)phenyl]thio]-β-propyl-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

- RN 852053-40-8 HCAPLUS
- CN Benzenepentanoic acid, β-amino-2-chloro-4-[[3-(phenylmethoxy)phenyl]thio]-β-2-propen-1-yl-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} & \text{O} - \text{CH}_2 - \text{Pl} \\ \text{H}_2\text{C} = \text{CH} - \text{CH}_2 - \text{C} - \text{CH}_2 - \text{CH}_2 \\ \text{HO}_2\text{C} - \text{CH}_2 \end{array}$$

- RN 852053-41-9 HCAPLUS
- CN Benzenepentanoic acid, β -amino-2-chloro- β -(3-hydroxypropyl)-4-[[3-(phenylmethoxy)phenyl]thio]-, hydrochloride (1:1) (CA INDEX NAME)

● HC1

- RN 852053-68-0 HCAPLUS
- CN Benzenepentanoic acid, 2-chloro-β-(hydroxymethyl)-β-(methylamio)-4-[[3-(phenylmethoxy)phenyl]thio]-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

N 852053-69-1 HCAPLUS

RN

CN Benzenepentanoic acid, 2-chloro-β-(hydroxymethyl)-β-(phenylamio)-4-[[3-(phenylmethoxy)phenyl]thio]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} & \text{C} \\ \text{NHPh} \\ \text{HO}_2\text{C}-\text{CH}_2-\text{C}-\text{CH}_2-\text{CH}_2 \\ \text{HO}-\text{CH}_2 \end{array}$$

- RN 852053-89-5 HCAPLUS
- CN Benzenepentanoic acid, β -amino-2-chloro- β -methyl-4-[[4-(phenylmethoxy)phenyl]thio]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} & \text{Me} \\ \text{HO}_2\text{C}-\text{CH}_2-\text{C}-\text{CH}_2-\text{CH}_2 \\ & \text{NH}_2 \end{array} \\ \text{O-CH}_2-\text{PI} \\ \end{array}$$

● HCl

- RN 852053-90-8 HCAPLUS
- CN Benzenepentanoic acid, β -amino-2-chloro-4-[[4-(phenylmethoxy)phenyl]thio]- β -propyl-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

- RN 852053-91-9 HCAPLUS
- CN Benzenepentanoic acid, β -amino-2-chloro- β -(3-hydroxypropyl)-4-[[4-(phenylmethoxy)phenyl]thio]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{NH}_2 \\ \text{HO- (CH}_2)_3 - \text{C-CH}_2 - \text{CH}_2 \\ \text{HO}_2\text{C-CH}_2 \end{array}$$

- RN 852054-08-1 HCAPLUS
- CN Benzenepentanoic acid, β-amino-2-chloro-β-(hydroxymethyl)-4-[[4-(phenylmethoxy)phenyl]thio]-, (+)- (CA INDEX NAME)

Rotation (+).

- RN 852054-10-5 HCAPLUS
- CN Benzenepentanoic acid, β-amino-2-chloro-β-(hydroxymethyl)-4-[[4-(phenylmethoxy)phenyl]thio]-, (-)- (CA INDEX NAME)

Rotation (-).

- RN 852054-12-7 HCAPLUS
- CN Benzenepentanoic acid, β -amino-2-chloro- β -(hydroxymethyl)-4-[[3-(phenylmethoxy)phenyl]thio]-, (-)- (CA INDEX NAME)

Rotation (-).

$$CO_{2H}$$
 C_{1} C_{2H} C

RN 852054-14-9 HCAPLUS

CN Benzenepentanoic acid, β-amino-2-chloro-β-(hydroxymethyl)-4-[[3-(phenylmethoxy)phenyl]thio]-, (+)- (CA INDEX NAME)

Rotation (+).

RN 852054-43-4 HCAPLUS

CN Benzenepentanoic acid, β-amino-2-chloro-β-(hydroxymethyl)-4-[(4-hydroxyphenyl)thio]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \text{NH}_2 \\ \text{HO}_2\text{C}-\text{CH}_2-\text{C}-\text{CH}_2-\text{CH}_2 \\ \text{HO}-\text{CH}_2 \end{array}$$

● HCl

RN 852054-45-6 HCAPLUS

CN Benzenepentanoic acid, β-amino-2-chloro-β-(hydroxymethyl)-4-[(4-methoxyphenyl)thio]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \text{NH}_2 \\ \text{HO}_2\text{C}-\text{CH}_2-\text{C}-\text{CH}_2-\text{CH}_2 \\ \text{HO}-\text{CH}_2 \end{array}$$

- RN 852054-46-7 HCAPLUS
- CN Benzenepentanoic acid, β-amino-2-chloro-4-[[4-(cyclohexylmethoxy)phenyl]thio]-β-(hydroxymethyl)-, hydrochloride (1:1) (CA INDEX NAME)

HC1

- RN 852054-48-9 HCAPLUS
- CN Benzenepentanoic acid, β-amino-4-[(4-butoxyphenyl)thio]-2-chloroβ-(hydroxymethyl)-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \text{NH}_2 \\ \text{HO}_2\text{C-CH}_2\text{--C-CH}_2\text{--CH}_2 \\ \text{HO-CH}_2 \end{array}$$

● HC1

- RN 852054-50-3 HCAPLUS
- CN Benzenepentanoic acid, β-amino-2-chloro-β-(hydroxymethyl)-4-[(4-phenoxyphenyl)thio]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \text{NH}_2 \\ \text{HO}_2\text{C}-\text{CH}_2-\text{C}-\text{CH}_2-\text{CH}_2 \\ \text{HO}-\text{CH}_2 \end{array} \\ \text{OPI}$$

● HC1

- RN 852054-52-5 HCAPLUS
- CN Benzenepentanoic acid, β-amino-2-chloro-β-(hydroxymethyl)-4-[[4-(phenoxymethyl)phenyl]thio]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \text{NH}_2 \\ \text{HO}_2\text{C}-\text{CH}_2-\text{C}-\text{CH}_2-\text{CH}_2 \\ \text{HO}-\text{CH}_2 \end{array}$$

● HC1

- RN 852054-84-3 HCAPLUS
- CN Benzenepentanoic acid, β-amino-2-chloro-β-(hydroxymethyl)-4-[(3-hydroxyphenyl)thio]-, hydrochloride (1:1) (CA INDEX NAME)

HC1

- RN 852054-86-5 HCAPLUS
- CN Benzenepentanoic acid, β-amino-2-chloro-β-(hydroxymethyl)-4-[(3-methoxyphenyl)thio]-, hydrochloride (1:1) (CA INDEX NAME)

- RN 852054-88-7 HCAPLUS CN Benzenepentanoic acid, β -amino-2-chloro-4-[[3-
 - (cyclohexylmethoxy)phenyl]thio]- β -(hydroxymethyl)-, hydrochloride (1:1) (CA INDEX NAME)

HC1

- RN 852054-91-2 HCAPLUS
- CN Benzenepentanoic acid, β-amino-4-[(3-butoxyphenyl)thio]-2-chloro-β-(hydroxymethyl)-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} & \text{CBu-n} \\ \text{NH}_2 & \text{HO}_2\text{C-CH}_2-\text{C-CH}_2-\text{CH}_2 \\ \text{HO-CH}_2 & \text{C-CH}_2 & \text{C-CH}_2 \end{array}$$

HCl

- RN 852054-93-4 HCAPLUS
- CN Benzenepentanoic acid, β-amino-2-chloro-β-(hydroxymethyl)-4-[(3-phenoxyphenyl)thio]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \text{NH}_2 \\ \text{HO}_2\text{C}-\text{CH}_2-\text{CH}_2-\text{CH}_2 \\ \text{HO}-\text{CH}_2 \end{array}$$

- RN 852054-95-6 HCAPLUS
- CN Benzenepentanoic acid, β-amino-4-([1,1'-biphenyl]-3-ylthio)-2-chloroβ-(hydroxymethyl)-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \text{NH}_2 \\ \text{HO}_2\text{C}-\text{CH}_2-\text{C}+\text{C}_2\\ \text{HO}-\text{CH}_2 \end{array}$$

HC1

- RN 852054-97-8 HCAPLUS
- CN Benzenepentanoic acid, β-amino-2-chloro-β-(hydroxymethyl)-4-[[3-(2-phenylethynyl)phenyl]thio]-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

- RN 852054-99-0 HCAPLUS
- CN Benzenepentanoic acid, β-amino-2-chloro-β-(hydroxymethyl)-4-[[3-(2-phenylethenyl)phenyl]thio]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} & \text{C2} \\ \text{NH}_2 \\ \text{HO}_2 \text{C} - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\ \text{HO} - \text{CH}_2 \end{array}$$

RN 852055-01-7 HCAPLUS

CN Benzenepentanoic acid, β -amino-2-chloro- β -(hydroxymethyl)-4-[[3-(2-phenylethyl)phenyl]thio]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \text{NH}_2 \\ \text{HO}_2\text{C}-\text{CH}_2-\text{CH}_2-\text{CH}_2 \\ \text{HO}-\text{CH}_2 \end{array}$$

● HCl

RN 852055-03-9 HCAPLUS

CN

Benzenepentanoic acid, β -amino-2-chloro- β -(hydroxymethyl)-4-[(3-(2-oxo-2-phenylacetyl)phenyl]thio]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \text{NH}_2 \\ \text{HO}_2\text{C}-\text{CH}_2-\text{C}-\text{CH}_2-\text{CH}_2 \\ \text{HO}-\text{CH}_2 \end{array}$$

HC1

RN 852055-05-1 HCAPLUS

CN Benzenepentanoic acid, 4-[(3-acetylphenyl)thio]-β-amino-2-chloro-β-(hydroxymethyl)-, hydrochloride (1:1) (CA INDEX NAME)

10591774

$$\begin{array}{c} \text{C1} & \text{Ac} \\ \text{NH}_2 & \text{S} & \text{HO}_2\text{C}-\text{CH}_2-\text{CH}_2-\text{CH}_2 \\ \text{HO}_-\text{CH}_2 & \text{HO}_-\text{CH}_2 & \text{S} \end{array}$$

● HCl

REFERENCE COUNT: 65 THERE ARE 65 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 2004:548899 HCAPLUS

DOCUMENT NUMBER: 141:243786

TITLE: Synthesis of optically active β-alkyl aspartate via [3,3] sigmatropic rearrangement of

α-acyloxytrialkylsilane

AUTHOR(S): Sakaguchi, Kazuhiko; Yamamoto, Masahiro; Kawamoto, Tetsuo; Yamada, Takeshi; Shinada, Tetsuro; Shimamoto,

Keiko; Ohfune, Yasufumi

CORPORATE SOURCE: Graduate School of Science, Department of Material Science, Osaka City University, Sugimoto, Sumiyoshi,

Osaka, 558-8585, Japan SOURCE: Tetrahedron Letters (2004), 45(30), 5869-5872

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:243786

AB The synthesis of four types of optically active β-carbon-substituted analogs of threo-β-hydroxy aspartate (THA) and a β-carbon-substituted analog of threo-β-benzyloxy aspartate (TBOA), which are potent blockers of excitatory amino acid transporters in

the mammalian central nervous system, via the chirality-transferring ester-enolate Claisen rearrangement of $\alpha\text{-acyloxytrialkylsilane}$ is described.

IT 749927-13-7P

RN

RI: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis of optically active β -alkyl aspartate as glutamate uptake inhibitors in mammalian central nervous system) 749927-13-7 HCAPLUS

CN L-Aspartic acid, 3-methyl-2-(2-phenylethyl)-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

REFERENCE COUNT:

29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 1996:376463 HCAPLUS

DOCUMENT NUMBER: 125 - 168594 125:31609a,31612a

ORIGINAL REFERENCE NO.:

TITLE:

Ethyl N-(diphenylmethylene)glycinate as anionic glycine equivalent. Monoalkylation, dialkylation and Michael additions under solid-liquid phase-transfer catalvsis

CORPORATE SOURCE:

SOURCE:

PUBLISHER: DOCUMENT TYPE:

AUTHOR(S):

LANGUAGE: OTHER SOURCE(S): Lopez, Anna; Moreno-Manas, Marcial; Pleixats, Roser; Roglans, Anna: Ezguerra, Jeus: Pedregal, Concepcion Dep. Chem., Univ. Autonoma Barcelona, Barcelona,

08193, Spain Tetrahedron (1996), 52(24), 8365-8386 CODEN: TETRAB; ISSN: 0040-4020

Journal English CASREACT 125:168594

Elsevier

HO2C H₂N

AB Et N-(diphenylmethylene)qlycinate undergoes monoalkylations, dialkylations and Michael addns. to ethylenic and acetylenic acceptors under appropriate solid-liquid phase transfer catalysis conditions. Further transformations of the α-disubstituted ketimines leads to α-alkylated aspartic and clutamic acid derivs, HO2CCH2C(NH2)(CO2H)(CH2)nPh and HO2CCH2CH2C(NH2) (CO2H) (CH2) nPh (n = 2, 3), to bicyclic amino acids or derivs. featuring pryazolone and isoxazolone moieties I and II, and to α-substituted (E)-3,4-dehydroglutamic acids. 180609-01-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (phase-transfer alkylation, dialkylation, and Michael addition reactions of (diphenylmethylene)glycinate as glycine anion synthon)

RN 180609-01-2 HCAPLUS

CN Aspartic acid, 2-(2-phenylethyl)-, hydrochloride (9CI) (CA INDEX NAME)

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● HC1

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STRUCTURE FILE UPDATES: 19 JUL 2009 HIGHEST RN 1165441-73-5 DICTIONARY FILE UPDATES: 19 JUL 2009 HIGHEST RN 1165441-73-5

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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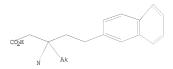
Uploading C:\Program Files\Stnexp\Queries\10591774b.str

chain nodes : 7 8 9 10 11 12 13 ring nodes : 1 2 3 4 5 6 15 16 17 18 chain bonds : 2-7 7-8 8-9 9-10 9-12 9-13 10-11 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 5-15 6-18 15-16 16-17 17-18 exact/norm bonds : 9-12 9-13 exact bonds : 2-7 7-8 8-9 9-10 10-11 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 5-15 6-18 15-16 16-17 17-18 isolated ring systems : containing 1:

Match level: 1:Atom 2:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom

L9 STRUCTURE UPLOADED

=> d 19 L9 HAS NO ANSWERS L9 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 19 SAMPLE SEARCH INITIATED 12:31:43 FILE 'REGISTRY'

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10591774

SAMPLE SCREEN SEARCH COMPLETED - 9 TO ITERATE

0 ANSWERS 100.0% PROCESSED 9 ITERATIONS SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE** 9 TO 360 PROJECTED ITERATIONS:

0 TO PROJECTED ANSWERS: 0

L10 0 SEA SSS SAM L9

=> s 19 sss full

FULL SEARCH INITIATED 12:31:50 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 206 TO ITERATE

100.0% PROCESSED 206 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

0 SEA SSS FUL L9 L11

=> log y

SINCE FILE TOTAL ENTRY SESSION 186.36 632.50 COST IN U.S. DOLLARS FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 0.00 -5.7 DISCOUNT AMOUNTS (FOR OUALIFYING ACCOUNTS) -5.74 CA SUBSCRIBER PRICE

STN INTERNATIONAL LOGOFF AT 12:32:25 ON 21 JUL 2009